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=> fil reg
FILE 'REGISTRY' ENTERED AT 15:30:29 ON 13 OCT 2004
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DICTIONARY FILE UPDATES:  12 OCT 2004  HIGHEST RN 761381-83-3

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

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http://www.cas.org/ONLINE/DBSS/registryss.html

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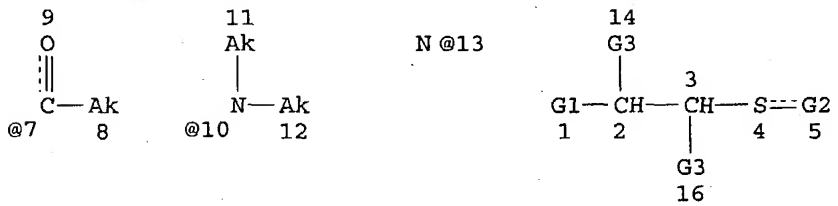


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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  14
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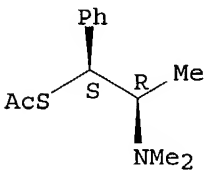
ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1965:8904 CAPLUS
DOCUMENT NUMBER: 62:8904
ORIGINAL REFERENCE NO.: 62:1588a-c
TITLE: Phenylmercaptoalkylamines. III. Hofmann degradation of 1-phenyl-2-dimethylaminopropanethiol quaternary salts
AUTHOR(S): Nishimura, Haruki; Takamatsu, Hideji
CORPORATE SOURCE: Dainippon Pharm. Co., Ltd., Osaka, Japan
SOURCE: Yakugaku Zasshi (1964), 84(9), 811-17
CODEN: YKKZAJ; ISSN: 0031-6903
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB Na2S2O3 and L-(+)-threo-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, followed by hydrolysis, gave (+)-1-phenyl-2-dimethylaminopropanethiol (I), which was then converted into the methiodide and treated with NaOH to form (+)-1,2-epithiopropylbenzene (II), b10 100°, which was polymerized to give a polymer, m. 255-6°. Treatment of D-(+)-erythro-1,2-epoxypropylbenzene with KSCN gave L-(-)-erythro-1,2-epithiopropylbenzene, b7 92-3°, [α]20D-21.4° (c 2.21, MeOH), which was found to be the antipode of II. II belongs to the D-(+)-erythro series and I, to the L-(+)-threo series. The (-)-amino thiol, similarly derived from L-(-)-erythro-N,N-dimethyl-1-chloro-1-phenyl-2-propylamine-HCl, was found to belong to the L-(-)-erythro series and that D-(+)-threo-1,2-epithiopropylbenzene (III) is derived from it. The steric configuration of II and III was also determined from their N.M.R. spectra. Hofmann degradation of the quaternary salt of 1-phenyl-2-dimethylaminoethanethiol also gave the same result. II and III underwent desulfurization by heating to give trans-β-methylstyrene.

IT **1210-30-6**, α-Toluenethiol, α-[1-(dimethylamino)ethyl]-, acetate (ester), L(-)-erythro-
(preparation of)
RN 1210-30-6 CAPLUS
CN Acetic acid, thio-, S-[α-[1-(dimethylamino)ethyl]benzyl] ester, erythro- (8CI) (CA INDEX NAME)

Relative stereochemistry.



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:497835 CAPLUS

DOCUMENT NUMBER: 131:350834

TITLE: Utilization of industrial waste materials. Part 14. Synthesis of β-amino alcohols and thiols with a 2-azabicyclo[3.3.0]octane backbone and their application in enantioselective catalysis

AUTHOR(S): Kossenjans, Michael; Soeberdt, Michael; Wallbaum, Sabine; Harms, Klaus; Martens, Jurgen; Aurich, Hans Gunter

CORPORATE SOURCE: Fachbereich Chemie, Universitat Oldenburg, Oldenburg, D-26129, Germany

SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (16), 2353-2365
CODEN: JCPRB4; ISSN: 0300-922X

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:350834

AB New, chiral β-tert-amino tert-alcs. were synthesized from an enantiomerically pure sec-amine via glycine, alanine and phenylglycine derivs. Grignard addns. to these esters provided rigid amino alcs. in fair yields. The absolute configurations of the stereogenic centers, which arose during the alkylation step, were assigned by an independent route leading to some of the optical antipodes. The target compds. were derivs. of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol. Condensation of enantiomerically pure β-amino alcs. with a γ-keto ester afforded N,O-acetals which were subsequently reduced to the β-tert-amino alcs. X-Ray anal. of one compound was performed to verify the stereochem. observed by chemical correlation. The nucleophilic ring opening of enantiomerically pure styrene oxide by an amine resulted in the formation of regioisomeric amino alcs. Amino thiol derivs. were also prepared Reduction of these compds. to thiols and subsequent oxidation afforded amino disulfides. Finally, the bicyclic β-amino alcs. and thiols were used as chiral ligands in the enantioselective addition of diethylzinc to benzaldehyde and ee values up to 96% were found.

IT **250371-17-6P**

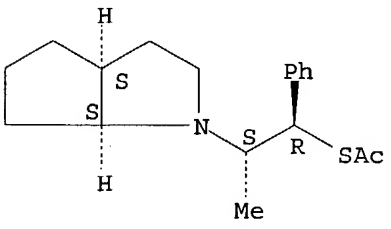
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of cyclopenta[b]pyrrole-1-ethanol and cyclopenta[b]pyrrole-1-ethanethiol derivs. as stereoselective addition catalysts)

RN 250371-17-6 CAPLUS

CN Ethanethioic acid, S-[(1R,2S)-2-[(3aS,6aS)-hexahydrocyclopenta[b]pyrrol-1(2H)-yl]-1-phenylpropyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



ANSWER 1 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

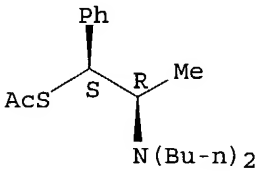
ACCESSION NUMBER: 1998:569540 CAPLUS
DOCUMENT NUMBER: 129:289723
TITLE: Zirconocene-Zinc Transmetalation and in Situ Catalytic Asymmetric Addition to Aldehydes
AUTHOR(S): Wipf, Peter; Ribe, Seth
CORPORATE SOURCE: Department of Chemistry, University of Pittsburgh, Pittsburgh, PA, 15260, USA
SOURCE: Journal of Organic Chemistry (1998), 63(19), 6454-6455
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The in situ hydrozirconation of alkynes, trans-metalation to dimethylzinc and chiral amino thiol-catalyzed addition to aldehydes provided an efficient protocol for the asym. preparation of (E)-allylic alcs. For example, the hydrozirconation of 1-hexyne, followed by transmetalation via addition of dimethylzinc and sequential addition of the resulting (alkenyl)methylzinc intermediate to benzaldehyde gave [S-(E)]-1-phenyl-2-hepten-1-ol [i.e., [S-(E)]-α-(1-hexenyl)benzenemethanol] in 90% and in 83% enantiomeric excess. The last step in the sequence was catalyzed in the presence of (R)-2-[1-(dimethylamino)propyl]benzenethiol as ligand.

IT **185606-94-4**
RL: CAT (Catalyst use); USES (Uses)
(preparation of allylic alcs. via hydrozirconation of alkynes and alkylzinc addition to aldehydes)

RN 185606-94-4 CAPLUS
CN Ethanethioic acid, S-[(1S,2R)-2-(dibutylamino)-1-phenylpropyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT:

ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

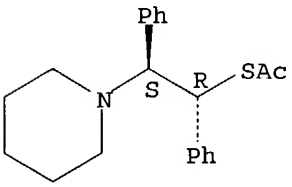
ACCESSION NUMBER: 1997:39785 CAPLUS
DOCUMENT NUMBER: 126:131036
TITLE: Chiral β-amino thiol catalysts for the enantioselective addition of diethylzinc to aldehydes
AUTHOR(S): Kang, Jahyo; Kim, Jeong Whan; Lee, Jun Won; Kim, Dong Soo; Kim, Joo In
CORPORATE SOURCE: Dep. Chem., Sogang Univ., Seoul, 121-742, S. Korea
SOURCE: Bulletin of the Korean Chemical Society (1996), 17(12), 1135-1142
CODEN: BKCSDE; ISSN: 0253-2964
PUBLISHER: Korean Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Reaction of diethylzinc with α-branched aldehydes in the presence of a catalytic amount (5 mol %) of various β-amino thiols in toluene or ether provided the corresponding secondary alcs. in outstanding ee. Detailed preparative procedure for the β-amino thiols are presented.

IT **160011-79-0P 166031-45-4P 166031-48-7P 186314-11-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(enantioselective addition of diethylzinc to aldehydes using chiral β-amino thiol catalysts)

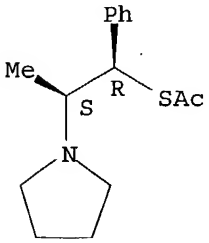
RN 160011-79-0 CAPLUS
CN Ethanethioic acid, S-[(1R,2S)-1,2-diphenyl-2-(1-piperidinyl)ethyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



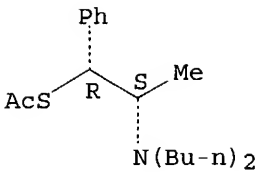
RN 166031-45-4 CAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-pyrrolidinyl)propyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



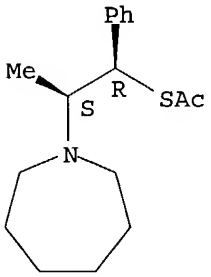
RN 166031-48-7 CAPLUS
CN Ethanethioic acid, S-[2-(dibutylamino)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



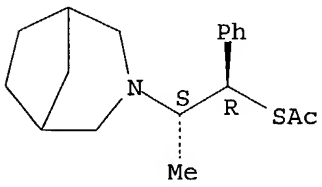
RN 186314-11-4 CAPLUS
CN Ethanethioic acid, S-[2-(hexahydro-1H-azepin-1-yl)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **186314-19-2P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective addition of diethylzinc to aldehydes using chiral β-amino thiol catalysts)
RN 186314-19-2 CAPLUS
CN Ethanethioic acid, S-[2-(3-azabicyclo[3.2.1]oct-3-yl)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 1 OF 1 CAPLUS COPYRIGHT 2004 ACS on STN

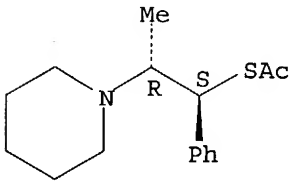
ACCESSION NUMBER: 1996:729946 CAPLUS
DOCUMENT NUMBER: 126:103872
TITLE: New chiral catalysts for the highly enantioselective addition of diethylzinc to aldehydes
AUTHOR(S): Jin, Myung-Jong; Ahn, Sum-Jin; Lee, Kyoung-Soo
CORPORATE SOURCE: Dep. Chemical Engineering, Inha Univ., Inchon, 402-751, S. Korea
SOURCE: Tetrahedron Letters (1996), 37(48), 8767-8770
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Optically active amino thioacetate derivs. of (+)-norephedrine were found to act as effective catalysts for enantioselective addition of diethylzinc to aldehydes. This reaction provided optically active secondary alcs. with e.e. of up to >99%.

IT **185606-97-7**
RL: CAT (Catalyst use); USES (Uses)
(chiral catalysts for enantioselective addition of diethylzinc to aldehydes)

RN 185606-97-7 CAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-piperidinyl)propyl] ester, [S-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 2 OF 2 CAPLUS COPYRIGHT 2004 ACS on STN

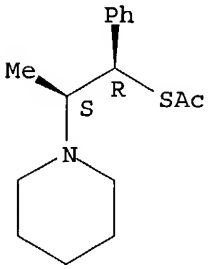
ACCESSION NUMBER: 1995:86424 CAPLUS
DOCUMENT NUMBER: 123:142957
TITLE: Enantioselective addition of diethylzinc to α-branched aldehydes
AUTHOR(S): Kang, Jahyo; Lee, Jun Won; Kim, Joo In
CORPORATE SOURCE: Department of Chemistry, Sogang University, Seoul, 121-742, S. Korea
SOURCE: Journal of the Chemical Society, Chemical Communications (1994), (17), 2009-10
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Reaction of diethylzinc with α-branched aldehydes in the presence of a catalytic amount of (1R,2S)-(-)-1-phenyl-2-piperidinopropane-1-thiol provided the corresponding secondary alcs. in almost 100% enantiomeric excess.

IT **166031-44-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthetic intermediate; in conversion to ligand catalyst for enantioselective addition of diethylzinc to α-branched aldehydes)

RN 166031-44-3 CAPLUS
CN Ethanethioic acid, S-[1-phenyl-2-(1-piperidinyl)propyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

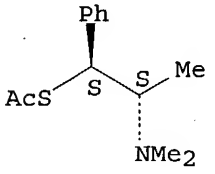
ACCESSION NUMBER: 1994:680925 CAPLUS
DOCUMENT NUMBER: 121:280925
TITLE: Nucleophilic substitutions using O-alkyl-N,N'-dialkylisoureas. Applications to ephedrines
AUTHOR(S): Poelert, Martin A.; Hulshof, L. A.; Kellogg, Richard M.
CORPORATE SOURCE: Dep. Organic Chemi., Univ. Groningen, Groningen, 9747 AG, Neth.
SOURCE: Recueil des Travaux Chimiques des Pays-Bas (1994), 113(7-8), 365-8
CODEN: RTCPA3; ISSN: 0165-0513
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:280925

AB Dialkylcarbodiimides in the presence of a CuI catalyst react cleanly with the hydroxyl group of N-methylated (1R,2S)-ephedrine and (1S,2S)-pseudoephedrine. These adducts react with nucleophiles like alkyl and aryl thiols as well as thioic acids and phthalimide to form the substitution products with overall retention of configuration. It is postulated that intramol. participation of the amino group via an SN2 reaction leads to aziridinium salts, which are subsequently opened by the nucleophiles via a second SN2 reaction. This synthetic approach is also useful for the inversion of simple secondary alcs.; on treatment with dicyclohexylcarbodiimide followed by benzothioic acid and treatment with LiAlH4, menthol was converted in good yield to neomenthane thiol.

IT **2226-22-4P 2226-23-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(nucleophilic substitutions using alkyldialkylisoureas, applications to ephedrines)

RN 2226-22-4 CAPLUS
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [S-(R*,R*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 2226-23-5 CAPLUS
CN Ethanethioic acid, S-[2-(dimethylamino)-1-phenylpropyl] ester, [R-(R*,S*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.